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Conformations of Single Semiflexible Chains in Poor Solvents

Density-of-States Monte Carlo Simulation

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1 Introduction

The conformational behavior of a single semiflexible chain has been investigated by using Monte Carlo simulations. In contrast to the continuous transition of a neutral flexible polymer, a semiflexible chain undergoes a discontinuous conformational transition, as solvent quality is decreased. Such a transition is analogous to the first-order phase transition, with coexistent elongated and compact conformational states. [1] In this work, computer simulations are carried out to manifest the elongated and compact conformational states for a short semiflexible chain.

2 Model

Here the semiflexible chain is modeled as a nonlinear elastic chain (FENE) of 8-mers, subjected to a bending energy due to local chain stiffness. [2] Also, monomers interact through a repulsive Lennard-Jones (L-J) potential to account for their excluded volume. The parameters are adopted from reference 2. To model poor solvents, an attractive Yukawa potential is incorporated between monomers, with an adjustable interaction strength ϵ. In the simulations, chain conformation is relaxed by using random walks for monomers, equivalent to monomer Brownian motion. [3]

3 Results and Discussion

Our simulations show that for smaller ϵ, chain conformation remains coiled-like, but for larger ϵ, chain tends to contract. Once chain reaches the folded state, a reverse process is applied to unfold chain conformation by decreasing ϵ in the simulations. A hysteresis loop for the folding-unfolding cycle of a stiff enough chain is observed. A further study is carried out via the density-of-states Monte Carlo method (DOSMC) [4] to discern the stability of the two different conformational states for a given ϵ in the hysteresis loop. We find that the energy distribution obtained from DOSMC is close to that of the folded state (in figure 1), indicating its thermodynamic stability.

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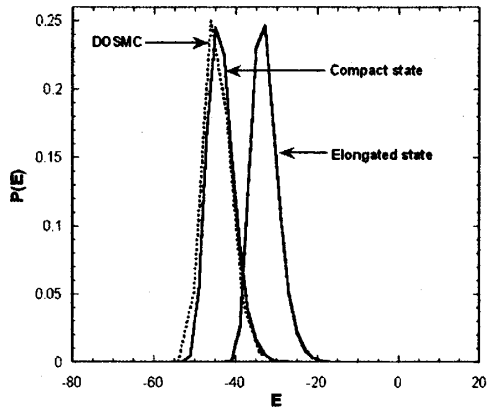

Figure 1: Comparison of the simulated energy distribution of elongated (unfolded) and compact (folded) conformational states (solid lines) with that of DOSMC (dotted line).

4 Conclusions

The conformational behavior of a short semiflexible chain is investigated by using Monte Carlo simulations. The traditional Monte Carlo method generates a conformational hysteresis loop for a stiff enough chain. The elongated and compact conformational states are dominated for the folding and unfolding processes, respectively. From the simulations of the density of states, we find that the folded state can be more favorable thermodynamically in the hysteresis loop.

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